

Fig. 1

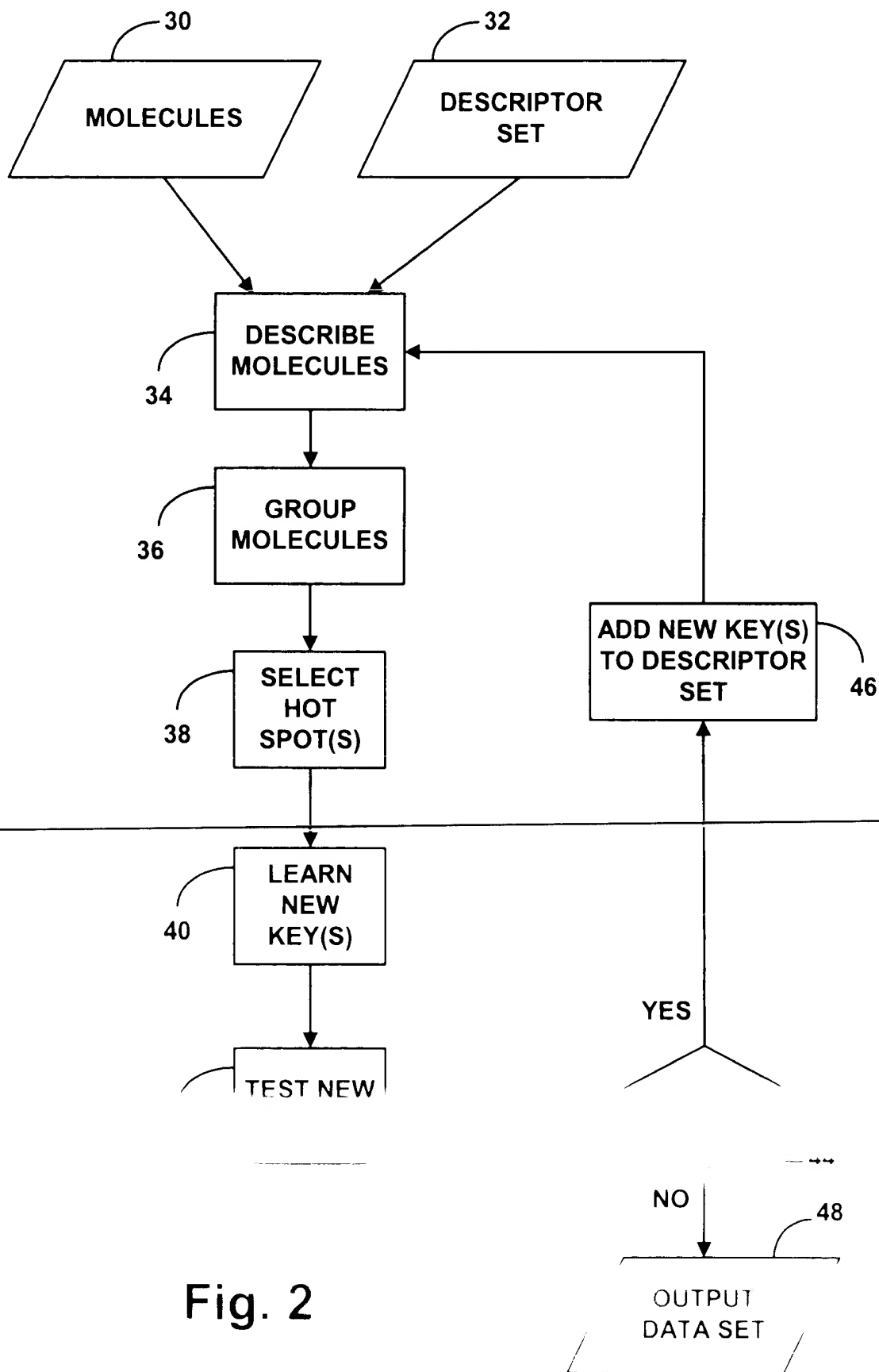


Fig. 2

Figure 3a

Exemplary Starting Keys			
SMARTS Query	Minimum hits	Weight	Comment and corresponding MACCS definition, if any
[R2;r5]~[R2;r5]	1	7	1 Any double ring, structure with the smallest ring a 5 member ring
[R2;r6]~[R2;r6]	1	7	2 Any double ring structure with the smallest ring a 6 member ring
[!#6;r4][r4][r4][r4]	1	100	3 QAAA@1
[#4,#12,#20,#38,#56,#88]	1	100	4 Group IIA
[r4]	1	100	5 4 M ring
[#29,#30,#47,#48,#79,#80]	1	95	6 group IB,IIB
[#8]~[#7]~[#6]~[#6]	1	100	7 ON(C)C
[#16]~[#16]	1	100	8 S-S
[#8]~[#6]~[#8]~[#8]	1	100	9 OC(O)O
[!#6]1~*~*1	1	100	10 QAA@1
C#C	1	85	11 CTC
[#5,#13,#31,#49,#81]	1	76	12 Group IIIA
[r7]	1	90	13 7 M ring
[#14]	1	40	14 Si
[#6]=[#6]~[#6]~[#6]	1	56	15 C=C(Q)Q
[r3]	1	80	16 3 M ring
[#7]~[#6]~[#8]~[#8]	1	18	17 NC(O)O
[#7]~[#8]	1	9	18 N-O
[#7]~[#6]~[#7]~[#7]	1	45	19 NC(N)N
[#6;R]=[#6;R](@*)@*	1	35	20 C\$=C(\$A)(\$A)
[#53]	1	40	21 I
[!#6][CH2][!#6]	1	57	22 OCH2O
[#15]	1	20	23 P
[#6]~[#6]~[#6]~[#6]~*	1	29	24 CQ(C)(C)A
[!#6]~[#9,#17,#35,#53]	1	23	25 QX
[#6]~[#16]~[#7]	1	50	26 CSN
[#7]~[#16]	1	46	27 NS
[CH2]=,.*	1	26	28 CH2=A
[#16;r]	1	30	29 S heterocycle
[#7]~[#6]~[#8]~[#7]	1	12	30 NC(O)N
[#7]~[#6]~[#6]~[#7]	1	20	31 NC(C)N
[#8]~[#16]~[#7]~[#7]	1	14	32 NC(C)C
[#9]	1	10	33 F
[!#6;H1,H2,H3]~*~[!#6;H1,H2,H3]	1	10	36 QHAQH
[#6]=[#6]~[#7]	1	14	37 C=CN
[#35]	1	14	38 Br
[#16]~*~*~*	1	14	39 SAN

Figure 1 illustrates a two-dimensional lattice structure. A central point is labeled i . To its right is a point labeled j . Above i is a point labeled $i-1$, and below i is a point labeled $i+1$. To the left of i is a point labeled $i-2$, and to the right of i is a point labeled $i+2$. The grid is bounded by dashed lines on the top and bottom, and solid lines on the left and right.

SMARTS Query	Minimum hits	Weight	Comment and corresponding MACCS definition, if any
[#8]~[!#6](~[#8])~[#8]	1	10	40 OQ(O)O
[-,-,-,+ ,++ ,+++]	1	6	41 charge
[#6]=[#6](~[#6])~[#6]	1	11	42 C=C(C)C
#6]~[#16]~[#8]	1	14	43 CSO
#7]~[#7]	1	12	44 NN
[!#6;H1,H2,H3]~*~*[!#6;H1,H2,H3]	1	10	45 QHAAAQH
[!#6;H1,H2,H3]~*~*[!#6;H1,H2,H3]	1	8	46 QAHAQH
[#8]~[#16]~[#8]	1	13	47 OSO
[#8]~[#7](~[#8])~[#6]	1	11	48 ON(O)C
#8;r]	1	8	49 O heterocycle
[!#6]~[#16]~[!#6]	1	12	50 QSQ
#16]:!*:	1	12	51 Snot%A%A
#16]=,:[#8]	1	13	52 S=O
~[#16](~)~*	1	12	53 AS(A)A
@*!@**	1	11	54 A\$A!A\$A
#7]=,:[#8]	1	11	55 N=O
@*!@[#16]	1	11	56 A\$A!S
#6]:[#7]	1	12	57 C%N
#6][#6]([#6])([#6])*	1	9	58 CC(C)(C)A
[!#6]~[#16]	1	11	59 QS
[!#6;H1,H2,H3]~[!#6;H1,H2,H3]	1	8	60 QHQH(&...)
[!#6]~[!#6;H1,H2,H3]	1	8	61 QQH
[!#6]~[#7]~[!#6]	1	9	62 QNQ
[#7]~[#8]	1	9	63 NO
[#8]~*~*~[#8]	1	7	64 OAAO
#16]=,*	1	8	65 S=A
#6H3]~*~[#6H3]	1	6	66 CH3ACH3
![#@7]@	1	8	67 A!N\$A
[#6]=[#6](~*)~*	1	6	68 C=C(A)A
[#7]~*~[#7]	1	5	69 NAN
[#6]=[#7]	1	6	70 C=N
[#7]~*~*~[#7]	1	6	71 NAAN
[!#6;!#1,r5]1~[r5]~[r5]~[r5]~[r5]1	1	5	75 QAAAA@1
[#7;H2,H3,H4]	1	6	76 NH2
[#6]~[#7](~[#6])~[#6]	1	5	77 CN(C)C
[#6;H2,H3]~[!#6]~[#6] H1,H2,H3]	1	6	78 CH2QQCH
#9 #17 #35 #53]1 * ! *	1	6	79 A\$A

Figure 3c

[illegible]

Figure 3d

Exemplary Starting Keys Cont.			
SMARTS Query	Minimum hits	Weight	Comment and corresponding MACCS definition, if any
@!@[#8]	2	2	119 A\$A!O > 1 & ...
[CH2]~*~*[CH2]*	1	3	120 ACH2AAACH2A
~[#6&H2]~~*~[#6&H2]~*	1	3	121 ACH2AACH2A
[!#6]~[!#6]	2	2	122 QQ > 1
[!#6,H1,H2,H3,H4]	2	2	123 QH > 1
[#8]~*[CH2]*	1	2	124 OACH2A
@!@[#7]	1	2	125 A\$A!N
[#9,#17,#35,#53]	1	2	126 X (halogen)
[#7]!.*.*	1	2	127 Nnot%A%A
[#8]=.*	2	2	128 O=A>1
[!#6&r]	1	3	129 heterocycle
[!#6]~[CH2]~*	2	2	130 QCH2A>1 & ...
[#8;H1,H2]	1	2	131 OH
[#8]	4	2	132 O > 3 and other features ..
[CH3]	3	2	133 CH3 > 2
[#7]	2	2	134 N>1
@!@[#8]	1	2	135 A\$A!O
!..*!.*	1	2	136 Anot%A%Anot%A
[r6]	7	2	137 6 M ring > 1
[#8]	3	2	138 O > 2
~[CH2]~[CH2]~	1	2	139 ACH2CH2A
~[!#6](~)~*	1	2	140 AQ(A)A
[CH3]	2	2	141 CH3 > 1
!@!@*!	1	2	142 A!A\$A!A
[#7;H1,H2,H3,H4]	1	2	143 NH
[#8]~[#6](~[#6])~[#6]	1	2	144 OC(C)C
[!#6][CH2]*	1	2	145 QCH2A
[#6]=.*O	1	1	146 C=O
!@[CH2]!@	1	1	147 A!CH2!A
[#7]~*(~*)~*	1	1	148 NA(A)A
[#6]-[#8]	1	1	149 C-O
[#6]-.[#7]	1	1	150 C-N
[#9]	1	1	151 O
[r6]	1	1	154 aromatic
[#8]	1	1	155 6 member ring
R	1	1	156 O
	1	1	157 ring

Fig. 4a

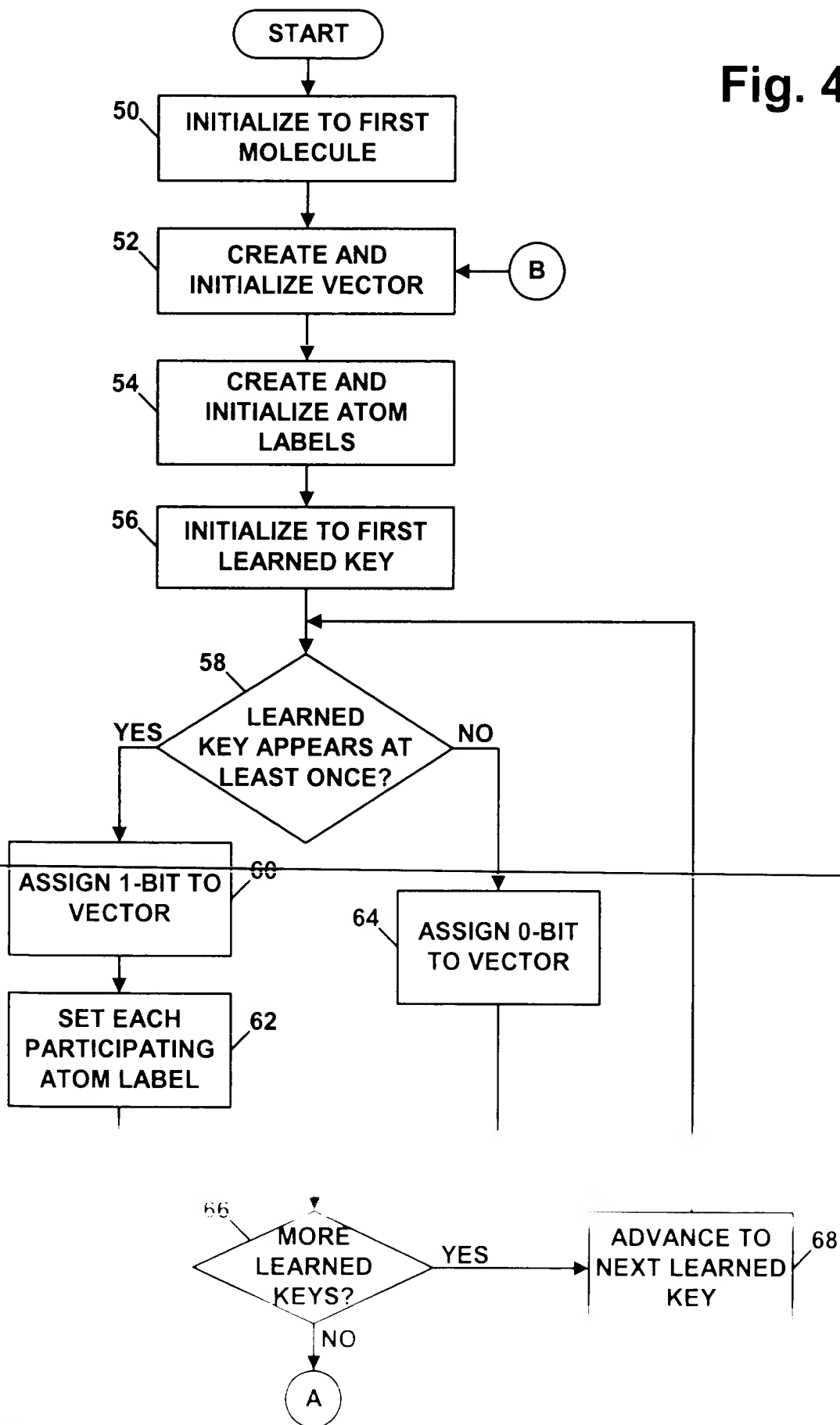
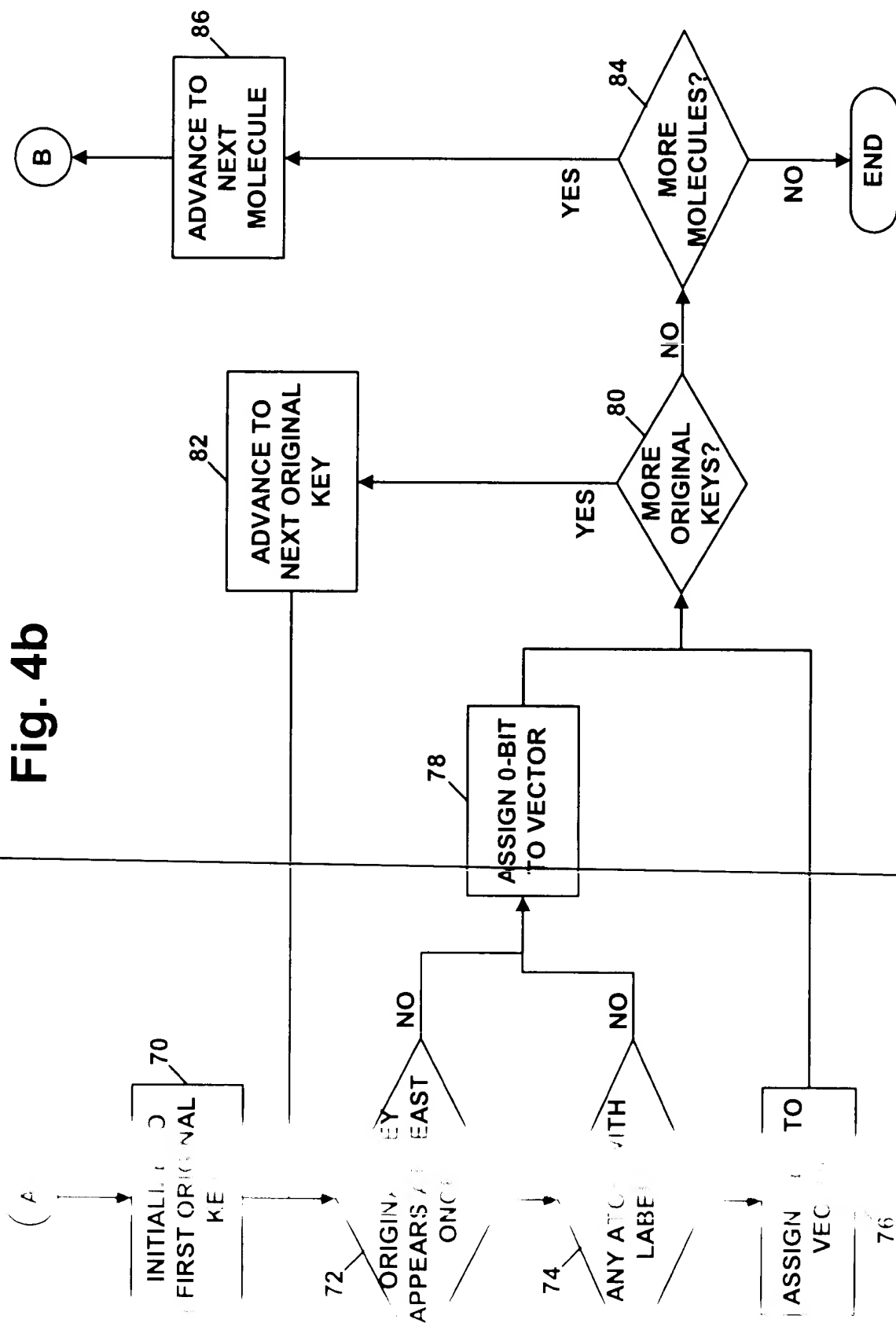


Fig. 4b



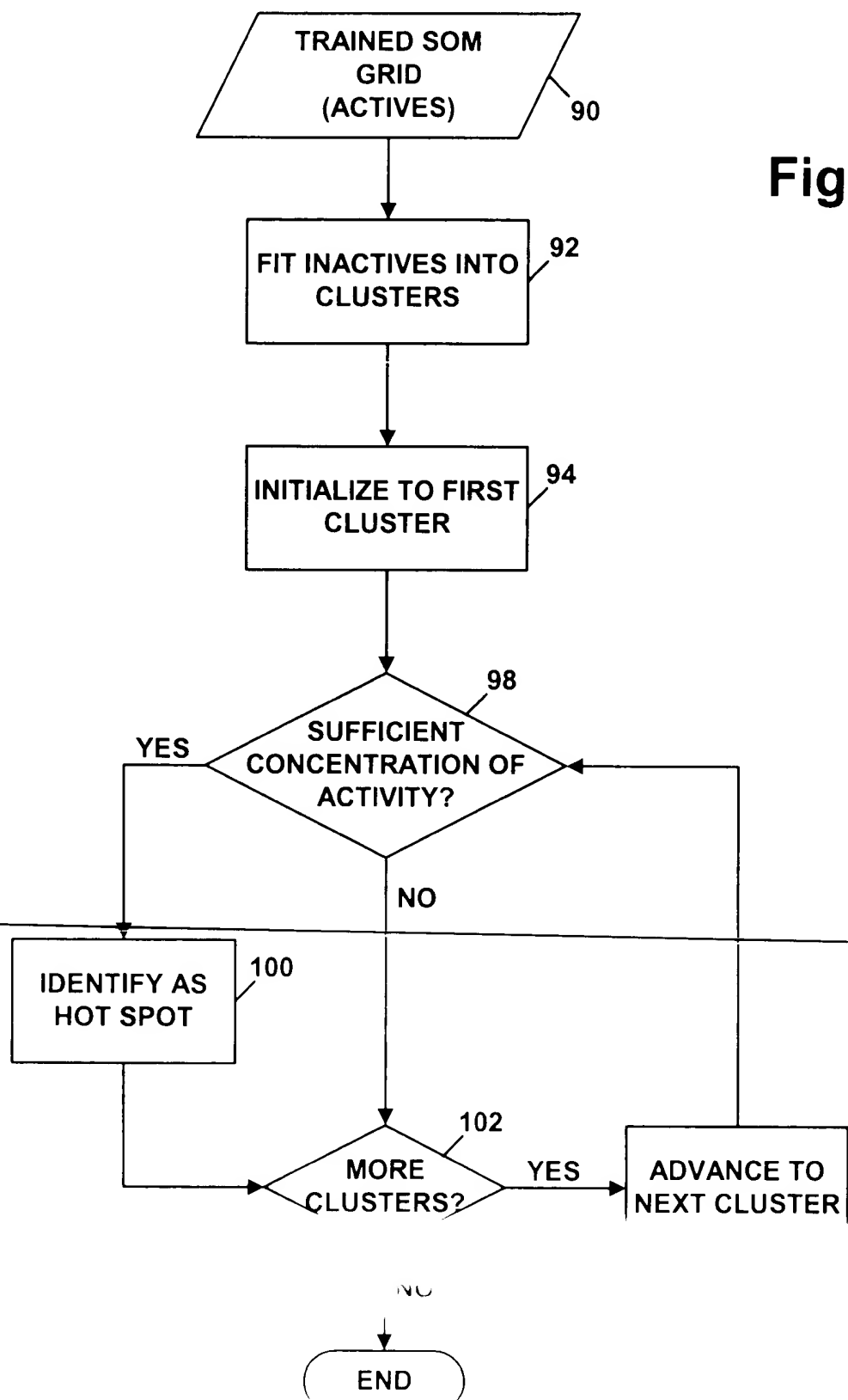


Fig. 6

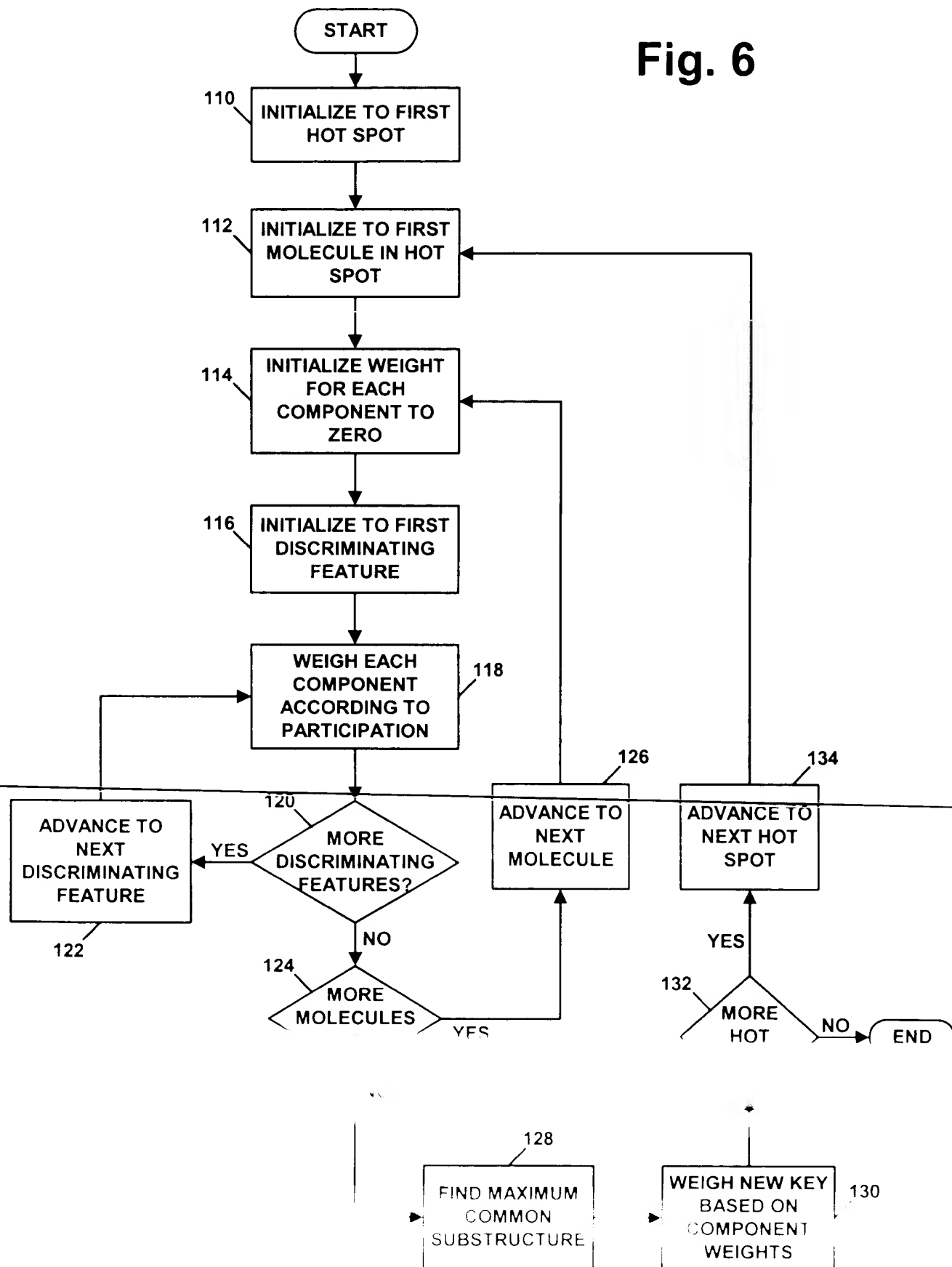


Fig. 7

